3,5-Dimethoxy-4-hydroxycinnamic acid

Other names:	Sinapinic acid
	Sinapic acid
	trans-3,5-Dimethoxy-4-hydroxycinnamic acid
	2-Propenoic acid, 3-(4-hydroxy-3,5-dimethoxyphenyl)-
	Cinnamic acid, 4-hydroxy-3,5-dimethoxy-
	4-Hydroxy-3,5-dimethoxycinnamic acid
Inchi:	InChI=1S/C11H12O5/c1-15-8-5-7(3-4-10(12)13)6-9(16-2)11(8)14/h3-6,14H,1-2H3,(H,12,
InchiKey:	PCMORTLOPMLEFB-ONEGZZNKSA-N
Formula:	C11H12O5
SMILES:	COc1cc(C=CC(=O)O)cc(OC)c1O
Mol. weight [g/mol]:	224.21
CAS:	530-59-6

Physical Properties

Property code	Value	Unit	Source
gf	-415.25	kJ/mol	Joback Method
hf	-646.12	kJ/mol	Joback Method
hfus	31.56	kJ/mol	Joback Method
hvap	84.90	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.507		Crippen Method
mcvol	162.840	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	763.39	K	Joback Method
tc	975.57	K	Joback Method
tf	527.04	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.85	J/mol×K	763.39	Joback Method
cpg	452.44	J/mol×K	798.75	Joback Method
cpg	461.52	J/mol×K	834.12	Joback Method

cpg	470.15	J/mol×K	869.48	Joback Method
cpg	478.36	J/mol×K	904.84	Joback Method
cpg	486.21	J/mol×K	940.21	Joback Method
cpg	493.72	J/mol×K	975.57	Joback Method
dvisc	0.0000663	Pa×s	527.04	Joback Method
dvisc	0.0000301	Pa×s	566.43	Joback Method
dvisc	0.0000152	Pa×s	605.82	Joback Method
dvisc	0.0000083	Pa×s	645.22	Joback Method
dvisc	0.0000049	Pa×s	684.61	Joback Method
dvisc	0.0000030	Pa×s	724.00	Joback Method
dvisc	0.0000020	Pa×s	763.39	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C530596&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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